ARKIV FÖR FYSIK Band 18 nr 1

Communicated 13 April 1960 by O. Klein and E. Rudberg

On the relativistic photoeffect in the *K*-shell

By Bengt C. H. Nagel

With 7 figures in the text

CONTENTS

Page
Introduction 1
1. The expression for the differential cross section, including polarizations 3
2. Initial and final state wave functions 6
3. Expansions of the reaction amplitudes in radial matrix elements . . 8
4. An approximate final state wave function in a Coulomb field. . . . 10
5. The reaction amplitudes to relative order αZ 13
6. Results and discussion 15
    a. Angular distribution, unpolarized photons 15
    b. Angular distribution, linearly polarized photons 16
    c. Electron polarization 17
    d. Total cross section 18
    e. The high-energy limit 19
7. Conclusions 20
Figs. 2–7 21
Appendix 23
References 27

SUMMARY

The relativistic *K*-shell photoeffect is analysed in terms of four "reaction amplitudes", which describe the process completely, including all polarization effects. Expansions of these amplitudes in radial matrix elements are given. Using an improvement of the Sommerfeld-Maue final state wave function, the amplitudes are computed to relative order αZ for a pure Coulomb field. Among effects obtained from the first-order terms are a non-zero forward emission intensity, and a transverse polarization of the photoelectrons, similar to that obtained in relativistic electron scattering.

Introduction

For a review of theoretical work in the atomic photoeffect up to about 1956—which in this context is practically equivalent to 1936— we refer to the article by Bethe and Salpeter in Handbuch der Physik XXXV (1957).

The theoretical interest in the photoeffect has been revived during the last years; this is to a large extent due to the more accurate experimental data on angular distribution of photoelectrons which have become available in the 50's, above all from the work of Hedgran, Hultberg and collaborators (see Hultberg 1959 and references there), who study the photoeffect as a means for indirect gamma-ray-spectroscopy, e.g. in the determination of internal conversion coefficients. New techniques for the study of electron and photon polarizations, partly inspired by the detection of parity violation in weak interactions, have made it of increased interest to investigate theoretically the polarization effects in the "classical" electron and photon processes. However, as far as the present author is aware, no experimental studies of electron polarization in the photoeffect have yet been reported.

The standard relativistic formula, valid in lowest order in αZ in a Coulomb field, for the angular distribution of K-shell photoelectrons from linearly polarized photons was derived by Sauter 1931. The correction of relative order αZ was recently obtained by Gavrila 1959. Electron polarizations have been studied theoretically in a number of papers: McVoy 1957, Olsen 1958, Banerjee 1958, 1959, and Fano, McVoy and Albers 1959. These authors in general work in the lowest order approximation, the same approximation that gives Sauter's expression for the differential cross section; however, Banerjee also obtained those terms of relative order αZ that survive in the high-energy limit. Concerning the total cross section we can mention—apart from the αZ-correction to Sauter's total cross section obtained in Gavrila's work—that the complete αZ-dependence in the high-energy limit has been worked out, mainly in papers by Erber 1959 and Pratt 1960.

In the present paper we try to analyse the K-shell photoeffect, including all polarization effects, in a way which can serve as a convenient starting point both for approximate analytic treatment and "exact" numerical calculations. Simple invariance arguments allow one to express the relevant matrix elements in four scalar "reaction amplitudes", which contain all information of the process; these amplitudes then seem to be a reasonable object for study.

The crucial point in the relativistic photoeffect is the final state wave function, describing the outgoing photoelectron; in the Dirac case this wave function can be obtained in exact form only as an infinite series of partial waves. With a view to numerical calculations the resulting expansions of the reaction amplitudes in radial electric and magnetic multipole moments are given. We then also derive expressions for these amplitudes to relative order αZ in a pure Coulomb field. The real parts of the αZ-terms give the correction of order αZ to Sauter's angular distribution, which was calculated by Gavrila. The imaginary αZ-terms give a new photoelectron polarization effect, a transverse polarization perpendicular to the scattering plane, obtained also when unpolarized photons are used. The imaginary terms also contribute to the forward and backward emission intensities in lowest non-vanishing order. We also get the αZ-corrections to the electron polarization effects obtained when the photons are circularly polarized.

Gavrila used in his work a final state wave function obtained by a second-order Born approximation. We proceed in a somewhat different way and use an improvement of the so-called Sommerfeld-Maue wave function; in this way we avoid the divergences that occur in second order when one applies the Born approximation to the Coulomb potential.

1. The expression for the differential cross section, including polarizations

The formula for the differential photoelectric cross section is generally derived by first-order time-dependent perturbation theory for the transition from an initial state, consisting of a photon with definite momentum and polarization and an electron in a bound state, to a final state in a continuum, consisting of a free electron with a definite asymptotic momentum. The electron states are taken to be one-electron states in the central field of the nucleus; the influence of the other electrons in the atom can be taken into account approximately by the use of a screened potential. The photon is either treated as a quantized field or, more elementary, as an external perturbation, harmonic in time, in the Hamiltonian of the electron. By standard procedure one then obtains the following expression for the differential cross section (= transition probability per unit time and unit solid angle, corresponding to an incident photon flux of one photon per unit time and unit area), assuming the electron to be described by the Dirac equation:

$$\sigma(i \to f;\, \hat{\mathbf{e}}) = \frac{1}{2\pi}\left(\frac{\hbar}{mc}\right)^2 \frac{e^2}{\hbar c}\,\frac{E}{h\nu}\,\frac{p}{mc}\left\{\left(\frac{mc}{\hbar}\right)^3 \left|\int \psi_f^*\, \boldsymbol{\alpha}\cdot\hat{\mathbf{e}}\, \exp\,(i\,\mathbf{k}\cdot\mathbf{r})\,\psi_i\, d\mathbf{r}\right|^2\right\}. \qquad (1.1)$$

Here $\mathbf{p}$ and $E = (m^2c^4 + c^2p^2)^{\frac{1}{2}}$ are momentum and relativistic energy of the outgoing electron, $\mathbf{k}$, $\hat{\mathbf{e}}$ and $h\nu$ momentum, polarization vector and energy of the photon. m and e are electron mass and charge, and $\boldsymbol{\alpha}$ stands for the Dirac matrices. ψ_i is the wave function of the bound electron, normalized to one,

$$\int \psi_i^*\,\psi_i\, d\mathbf{r} = 1. \qquad (1.2)$$

ψ_f is the final state wave function, an incoming scattering state with asymptotic form

$$(\exp\,(i\,\mathbf{p}\cdot\mathbf{r}) + \text{inc. spher. wave})\,w. \qquad (1.3)$$

w is a constant 4-spinor, with $w^* w = 1$. For simplicity we suppress the logarithmic term in the asymptotic plane wave exponent that occurs in the case of a Coulomb field.

That an incoming (and not an outgoing) scattering state must be used is due to the fact that only a superposition of such states gives for large positive times a plane wave packet (without spherical part), describing the photoelectron that moves away from the atom in a definite direction. (See Bethe and Salpeter 1957, p. 382, and references there.)

The factor $(mc/\hbar)^3$ in the brackets in (1.1) is inserted to make this part of the expression dimensionless. From now on we shall put $m = \hbar = c = 1$, i.e. we use $\hbar/mc$, mc and mc^2 as units of length, momentum and energy.

(1.1) refers to the transition between definite initial and final spin states of the electron under absorption of a photon with a definite polarization. To obtain the observed cross section we must perform a suitable averaging and summing over initial and final state polarizations. We shall give the cross section for a general initial photon polarization and a general polarization sensitivity of the detector of the photoelectrons. We will not assume the polarization of the bound electron to be observed, though this should in principle be possible, e.g. by studying the polarization of the X-ray emitted when the hole in the shell

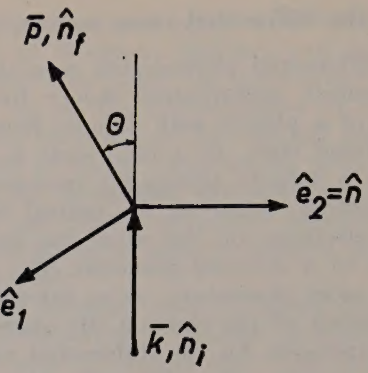

Fig. 1.

is filled up; it is, however, not difficult to generalize the intensity formula to include also this case. Polarization states of electrons and photons are conveniently described by 2×2 density matrices and parameters related to these matrices. We refer to Tolhoek 1956, whose notations we shall follow, for a good review of this formalism. Before applying this technique to our case, we must study the spin and photon polarization dependence of the matrix element.

We assume the initial state to be a $S_{\frac{1}{2}}$-state, e.g. a K-shell state. Then both the initial and final states of the electron are specified by giving the large component 2-spinors u_i and u_f. (See Tolhoek, loc. cit., p. 279, for a discussion of this way of describing the spin state of a relativistic electron.) For the final state, u_f means the constant 2-spinor of the asymptotic plane wave part. We may then write, observing that ψ_i and ψ_f are linear in u_i and u_f, respectively,

$$\int \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{e}} \exp(i \mathbf{k} \cdot \mathbf{r}) \psi_i \, d\mathbf{r} = u_f^* M(\hat{\mathbf{e}}) u_i, \tag{1.4}$$

where $M(\hat{\mathbf{e}})$ is a linear operator in spin space, and can thus be written as a linear combination of the unit matrix and Pauli spin matrices. $M(\hat{\mathbf{e}})$ depends linearly on $\hat{\mathbf{e}}$.

Introduce unit vectors $\hat{\mathbf{n}}_i$ and $\hat{\mathbf{n}}_f$ in the photon and electron directions (see Fig. 1). θ is the angle between $\hat{\mathbf{n}}_i$ and $\hat{\mathbf{n}}_f$. $\hat{\mathbf{n}} = \dfrac{\hat{\mathbf{n}}_i \times \hat{\mathbf{n}}_f}{|\hat{\mathbf{n}}_i \times \hat{\mathbf{n}}_f|}$ is the normal to the scattering plane. As basic photon polarization directions we choose $\hat{\mathbf{e}}_1$ in the scattering plane and $\hat{\mathbf{e}}_2 = \hat{\mathbf{n}}$, so that $\hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2 = \hat{\mathbf{n}}_i$.

The structure of $M(\hat{\mathbf{e}})$ is obtained by observing that if the electron moves in a central potential the matrix element (1.4) must be invariant under reflection in the scattering plane,

$$u_{fR}^* M(\hat{\mathbf{e}}_R) u_{iR} = u_f^* M(\hat{\mathbf{e}}) u_i. \tag{1.5}$$

Here $\hat{\mathbf{e}}_R$ is obtained from $\hat{\mathbf{e}}$ by changing the sign of the component along $\hat{\mathbf{e}}_2$, and $u_R = \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} u$, apart from an irrelevant phase-factor.

Then we get from (1.5)

$$\begin{aligned} M_1 &= M(\hat{\mathbf{e}}_1) = A(\theta) + i B(\theta) \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}, \\ M_2 &= M(\hat{\mathbf{e}}_2) = i C(\theta) \boldsymbol{\sigma} \cdot (\hat{\mathbf{n}} \times \hat{\mathbf{n}}_f) + i D(\theta) \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}_f. \end{aligned} \tag{1.6}$$

A, B, C and D, the "reaction amplitudes", are complex-valued scalar functions. The factors i are inserted for later convenience to give the same phase to the functions in the lowest order expressions for a Coulomb field.

If $\theta=0$, i.e. $\hat{\mathfrak{n}}_i=\hat{\mathfrak{n}}_f$ (then we define the scattering plane by $\hat{\mathfrak{n}}=\hat{\mathfrak{e}}_2$), M_2 is obtained from M_1 by a rotation $\pi/2$ around $\hat{\mathfrak{n}}_i$. This gives

$$A(0)=D(0)=0;\quad B(0)=-C(0). \tag{1.7}$$

Similarly

$$A(\pi)=D(\pi)=0;\quad B(\pi)=C(\pi). \tag{1.8}$$

Let us now return to the derivation of the intensity formula. Put $\hat{\mathfrak{e}}=a_1\hat{\mathfrak{e}}_1+a_2\hat{\mathfrak{e}}_2$, where $|a_1|^2+|a_2|^2=1$, and assume the detector of the photoelectrons to respond to the electron spin state according to $\varrho_{\text{det}}=\frac{1}{2}(1+\boldsymbol{\zeta}\cdot\boldsymbol{\sigma})$. Averaging over initial electron spin states (factor $\frac{1}{2}$ in (1.9)) we obtain the following expression which comes in instead of the brackets in (1.1) in the general formula:

$$\tfrac{1}{2}\,\text{Trace}\,(\varrho_{\text{det}}\,M(\hat{\mathfrak{e}})\,M^*(\hat{\mathfrak{e}})). \tag{1.9}$$

We now insert $M(\hat{\mathfrak{e}})=a_1M_1+a_2M_2$ and the expressions (1.6) into (1.9); instead of the resulting bilinear expressions in a_1 and a_2 we introduce the parameters

$$\xi_1=|a_1|^2-|a_2|^2;\quad \xi_2=a_1a_2^*+a_2a_1^*;\quad \xi_3=i(a_1a_2^*-a_2a_1^*). \tag{1.10}$$

The result of the trace calculation in (1.9), combined with (1.1), can then be expressed as

$$\sigma(\theta,\boldsymbol{\zeta},\boldsymbol{\xi})=C'K(\boldsymbol{\zeta},\boldsymbol{\xi}), \tag{1.11}$$

with

$$C'=\frac{1}{2\pi}\left(\frac{\hbar}{mc}\right)^2\frac{e^2}{\hbar c}\frac{E}{h\nu}\frac{p}{mc}, \tag{1.12}$$

and

$$\begin{aligned}2K(\boldsymbol{\zeta},\boldsymbol{\xi})=&\tfrac{1}{2}(|A|^2+|B|^2+|C|^2+|D|^2)+\text{Im}\,(AB^*+CD^*)\,\boldsymbol{\zeta}\cdot\hat{\mathfrak{n}}\\&+\xi_1[\tfrac{1}{2}(|A|^2+|B|^2-|C|^2-|D|^2)+\text{Im}\,(AB^*-CD^*)\,\boldsymbol{\zeta}\cdot\hat{\mathfrak{n}}]\\&+\xi_2[\text{Im}\,(AC^*-BD^*)\,\boldsymbol{\zeta}\cdot(\hat{\mathfrak{n}}\times\hat{\mathfrak{n}}_f)+\text{Im}\,(AD^*+BC^*)\,\boldsymbol{\zeta}\cdot\hat{\mathfrak{n}}_f]\\&+\xi_3[-\text{Re}\,(AC^*-BD^*)\,\boldsymbol{\zeta}\cdot(\hat{\mathfrak{n}}\times\hat{\mathfrak{n}}_f)-\text{Re}\,(AD^*+BC^*)\,\boldsymbol{\zeta}\cdot\hat{\mathfrak{n}}_f].\end{aligned} \tag{1.13}$$

(1.13) was derived assuming a complete polarization of the photon, i.e. $|\boldsymbol{\xi}|=1$, but it is easy to see that the formula is also valid for a partial polarization $|\boldsymbol{\xi}|<1$. Any 2×2 density matrix ϱ can be written $\varrho=\lambda_1\varrho_1+\lambda_2\varrho_2$, where λ_1, $\lambda_2\geqslant 0$, $\lambda_1+\lambda_2=1$, and ϱ_1 and ϱ_2 correspond to pure states (complete polarization). Speaking more physically: any statistical mixture can be obtained by incoherent superposition of two appropriately chosen pure states. The intensity of photoelectrons obtained from this incoherent superposition of photon polarization states is obtained by forming the same linear combination of the intensities corresponding to pure polarization states, and (1.13) is then valid also in the general case; the linear combination of the density matrices amounts to forming the same linear combination of the vectors $\boldsymbol{\xi}$.

It should be stressed that (1.11) gives the cross section per electron; multiplication by two gives the cross section for the K-shell.

We shall now look at some special cases of (1.11)–(1.13).

If the incident photons are linearly polarized, the angle between the polarization plane and the scattering plane being ϕ, and the final electron polarization is not observed (the detector accepts all electron polarizations), we should put $\hat{\mathbf{e}} = \cos\phi\,\hat{\mathbf{e}}_1 - \sin\phi\,\hat{\mathbf{e}}_2$, i.e. $\xi_1 = \cos 2\phi$, $\xi_2 = -\sin 2\phi$, and $\xi_3 = 0$, and add $K(\boldsymbol{\zeta}, \boldsymbol{\xi})$ and $K(-\boldsymbol{\zeta}, \boldsymbol{\xi})$. This gives

$$\sigma(\theta, \phi) = C' \{|C|^2 + |D|^2 + \cos^2\phi\,[|A|^2 + |B|^2 - |C|^2 - |D|^2]\}. \tag{1.14}$$

Unpolarized photons correspond to $\boldsymbol{\xi} = 0$:

$$\sigma(\theta) = C'\,\tfrac{1}{2}\{|A|^2 + |B|^2 + |C|^2 + |D|^2\}. \tag{1.15}$$

The same differential cross section is obtained also for circularly polarized photons, $\xi_1 = \xi_2 = 0$.

The polarization $\mathbf{P}$ of the outgoing photoelectrons, related to the density matrix by $\varrho = \tfrac{1}{2}(1 + \mathbf{P}\cdot\boldsymbol{\sigma})$, is obtained from the relation

$$\mathbf{P}\cdot\boldsymbol{\zeta} = \frac{K(\boldsymbol{\zeta}, \boldsymbol{\xi}) - K(-\boldsymbol{\zeta}, \boldsymbol{\xi})}{K(\boldsymbol{\zeta}, \boldsymbol{\xi}) + K(-\boldsymbol{\zeta}, \boldsymbol{\xi})}. \tag{1.16}$$

We will give $\mathbf{P}$ only for the case which is probably of greatest experimental interest, namely when the photons are (partially) circularly polarized, $\xi_1 = \xi_2 = 0$, $\xi_3 = P_\gamma$. $P_\gamma = 1\,(-1)$ corresponds to photon helicity $+1\,(-1)$, i.e. right (left) hand circular polarization, $P_\gamma = 0$ to unpolarized photons. From (1.13) and (1.16) we get

$$\mathbf{P} = P_1\,\hat{\mathbf{n}} + P_\gamma\,(P_2\,\hat{\mathbf{n}}_f + P_3\,\hat{\mathbf{n}}_f \times \hat{\mathbf{n}}), \tag{1.17}$$

with

$$P_1 = \frac{2\,\mathrm{Im}\,(A B^* + C D^*)}{|A|^2 + |B|^2 + |C|^2 + |D|^2}, \tag{1.18}$$

$$P_2 = -\frac{2\,\mathrm{Re}\,(A D^* + B C^*)}{|A|^2 + |B|^2 + |C|^2 + |D|^2}, \tag{1.19}$$

$$P_3 = \frac{2\,\mathrm{Re}\,(A C^* - B D^*)}{|A|^2 + |B|^2 + |C|^2 + |D|^2}. \tag{1.20}$$

P_1 is a transverse polarization, perpendicular to the scattering plane, and is obtained also for unpolarized photons; P_2 and P_3 are longitudinal and transverse polarizations in the scattering plane, and are obtained for circularly polarized photons.

2. Initial and final state wave functions

In this section we shall study the spin structure of ψ_i and ψ_f and give integral expressions for A, B, C and D.

ψ_i and ψ_f are solutions of the Dirac equation

$$[-i\,\boldsymbol{\alpha}\cdot\mathrm{grad} + \alpha_m + V(r) - \varepsilon]\,\psi = 0. \tag{2.1}$$

$\boldsymbol{\alpha}$, α_m are the four Dirac matrices, ε is the energy (in units mc^2). The α-matrices will be written as direct products of ϱ- and σ-matrices (see Dirac 1947, p. 255), and correspondingly the 4-spinor space will be considered as a direct product of "spin space", spanned by u_+ and u_-, and "large and small component space", spanned by v_+ and v_-. The σ-matrices operate on u, the ϱ-matrices on v. Thus e.g. $v_- u_+$ stands for the 4-spinor $(0, 0, 1, 0)$.

The initial $S_{\frac{1}{2}}$-state wave function ψ_i has the form

$$\psi_i = [g_i(r)\, v_+ - i\, f_i(r)\, \boldsymbol{\sigma}\cdot\hat{\mathbf{r}}\, v_-]\, u_i, \tag{2.2}$$

with normalization

$$4\pi \int_0^\infty [g_i^2 + f_i^2]\, r^2\, dr = 1; \quad u_i^* u_i = 1. \tag{2.3}$$

For the final state wave function we choose the z-axis as the direction of $\mathbf{p}$. ψ_f then has the asymptotic form (cf. (1.3))

$$\left(\frac{\varepsilon+1}{2\varepsilon}\right)^{\frac{1}{2}} [e^{ipz} + \text{inc. spher. wave}] \left(v_+ + \frac{p}{\varepsilon+1}\,\sigma_z v_-\right) u_f. \tag{2.4}$$

From the symmetry property of the scattering problem (2.1) and (2.4) under rotations around the z-axis and reflection in a plane containing the z-axis it follows (see Nagel 1960, Sect. 4) that ψ_f is of the form

$$\psi_f = \{[f_+(r,\vartheta) - i\, g_+(r,\vartheta)\, \sigma_\varphi]\, v_+ + [f_-(r,\vartheta) - i\, g_-(r,\vartheta)\, \sigma_\varphi]\, \sigma_z v_-\}\, u_f, \tag{2.5}$$

where

$$\sigma_\varphi = -\sin\varphi\, \sigma_x + \cos\varphi\, \sigma_y. \tag{2.6}$$

(The use of f and g in (2.2) and (2.5) is somewhat disturbing from the logical point of view, but the notation g and f in (2.2) for the large and small radial components is standard, and $f_\pm$ and $g_\pm$ in (2.5) are in a natural way connected with the scattering amplitudes $f(\vartheta)$ and $g(\vartheta)$ in Dirac scattering theory.)

Having chosen $\mathbf{p} = p\,\hat{\mathbf{z}}$, we now put $\mathbf{k} = k\,|-\sin\theta,\ 0,\ \cos\theta|$; then we also have $\hat{\mathbf{e}}_1 = |\cos\theta,\ 0,\ \sin\theta|$ and $\hat{\mathbf{e}}_2 = \hat{\mathbf{n}} = \hat{\mathbf{y}}$.

Inserting (2.2) and (2.5) into (1.4) and comparing with (1.6), we obtain expressions for A, B, C and D as integrals over g_i, f_i, $f_\pm$ and $g_\pm$. The calculations can be simplified by using trace techniques and the known forms (1.6). The result is

$$\begin{aligned} A(\theta) &= (\ \ I_2 + I_4 - I_7)\cos\theta + (I_1 - I_5 + I_6)\sin\theta \\ B(\theta) &= (-I_1 + I_3 + I_6)\cos\theta + (I_2 + I_4 + I_7)\sin\theta \\ C(\theta) &= \quad I_1 + I_3 - I_6 \\ D(\theta) &= -I_2 + I_4 - I_7. \end{aligned} \tag{2.7}$$

Here $I_1 \ldots I_7$ are the integrals

$$\begin{aligned}
I_1 &= -i\int f_+^* f_i \exp(i\mathbf{k}\cdot\mathbf{r}) \cos\vartheta \, d\mathbf{r}\\
I_2 &= -i\int f_+^* f_i \exp(i\mathbf{k}\cdot\mathbf{r}) \sin\vartheta \cos\varphi \, d\mathbf{r}\\
I_3 &= -i\int g_+^* f_i \exp(i\mathbf{k}\cdot\mathbf{r}) \sin\vartheta \cos 2\varphi \, d\mathbf{r}\\
I_4 &= -i\int g_+^* f_i \exp(i\mathbf{k}\cdot\mathbf{r}) \cos\vartheta \cos\varphi \, d\mathbf{r}\\
I_5 &= -i\int g_+^* f_i \exp(i\mathbf{k}\cdot\mathbf{r}) \sin\vartheta \, d\mathbf{r}\\
I_6 &= \int f_-^* g_i \exp(i\mathbf{k}\cdot\mathbf{r}) \, d\mathbf{r}\\
I_7 &= -\int g_-^* g_i \exp(i\mathbf{k}\cdot\mathbf{r}) \cos\varphi \, d\mathbf{r}.
\end{aligned} \tag{2.8}$$

3. Expansions of the reaction amplitudes in radial matrix elements

As is well-known, the exact final state wave function ψ_f cannot, even for a pure Coulomb field, be obtained in closed form in the Dirac case. One must use a partial waves expansion, and the reaction amplitudes are then obtained as series of (ordinary and associated) Legendre polynomials, with certain combinations of radial matrix elements as coefficients. We shall give these expansions here for future reference, although they will not be used in the following sections of this paper.

It turns out that the expansions in question are simpler if we choose instead of B, C and D certain linear combinations, which are related to the circular polarization states $\mathbf{e}_\pm = \hat{\mathbf{e}}_1 \pm i\,\hat{\mathbf{e}}_2$ (photon states of definite helicity) and also relate the electron spin to the direction of the photon instead of the outgoing electron. Introduce

$$M_\pm = M_1 \pm i\, M_2; \quad \sigma_\pm = \boldsymbol{\sigma}\cdot\mathbf{e}_\pm, \; \sigma_{//} = \boldsymbol{\sigma}\cdot(\hat{\mathbf{e}}_1\times\hat{\mathbf{e}}_2). \tag{3.1}$$

Then we have from (1.6)

$$\begin{aligned}
M_+ &= A(\theta) + E(\theta)\,\sigma_{//} + F(\theta)\,\sigma_+ + G(\theta)\,\sigma_-,\\
M_- &= A(\theta) - E(\theta)\,\sigma_{//} - G(\theta)\,\sigma_+ - F(\theta)\,\sigma_-,
\end{aligned} \tag{3.2}$$

where

$$\begin{aligned}
E(\theta) &= \sin\theta\, C(\theta) - \cos\theta\, D(\theta),\\
F(\theta) &= \tfrac{1}{2}\left[B(\theta) - \cos\theta\, C(\theta) - \sin\theta\, D(\theta)\right],\\
G(\theta) &= -\tfrac{1}{2}\left[B(\theta) + \cos\theta\, C(\theta) + \sin\theta\, D(\theta)\right].
\end{aligned} \tag{3.3}$$

The expansion of ψ_f, fulfilling the asymptotic condition (2.4), is obtained in the usual way by taking an expansion, with undetermined coefficients, in partial wave solutions obtained after separating the Dirac equation in spherical coordinates, and determining the coefficients so that after subtraction of the expansion of the plane wave part in (2.4) the rest only contains asymptotically incoming waves e^{-ipr}. Comparison with (2.5) then gives the following series for $f_\pm$ and $g_\pm$:

$$
\begin{aligned}
f_+(r,\vartheta) &= \sum i^l\,[l\,e^{-i\eta_l}\,g_l+(l+1)\,e^{-i\eta_{-l-1}}\,g_{-l-1}]\,P_l(\cos\vartheta),\\
g_+(r,\vartheta) &= \sum i^l\,[e^{-i\eta_l}\,g_l-e^{-i\eta_{-l-1}}\,g_{-l-1}]\,P_l^1(\cos\vartheta),\\
f_-(r,\vartheta) &= \sum i^l\,[(l+1)\,e^{-i\eta_{l+1}}\,f_{l+1}-l\,e^{-i\eta_{-l}}\,f_{-l}]\,P_l(\cos\vartheta),\\
g_-(r,\vartheta) &= \sum i^l\,[-e^{-i\eta_{l+1}}\,f_{l+1}-e^{-i\eta_{-l}}\,f_{-l}]\,P_l^1(\cos\vartheta).
\end{aligned}
\tag{3.4}
$$

g_n and f_n ($n=l$ or $-l-1$) are the ordinary large and small component radial wave functions, with asymptotic normalization

$$
\begin{aligned}
g_n &\approx \left(\frac{\varepsilon+1}{2\varepsilon}\right)^{\frac{1}{2}}\frac{1}{pr}\sin\left(pr-\frac{l\pi}{2}+\varkappa\ln 2pr+\eta_n\right),\\
f_n &\approx \left(\frac{\varepsilon-1}{2\varepsilon}\right)^{\frac{1}{2}}\frac{1}{pr}\cos\left(pr-\frac{l\pi}{2}+\varkappa\ln 2pr+\eta_n\right),
\end{aligned}
\tag{3.5}
$$

where η_n are the asymptotic phases, and (if we have a Coulomb potential present) $\varkappa=\alpha Z/\beta$, $\alpha=e^2/\hbar c$, $\beta=v/c$.

Introducing (2.2), (3.4) and the expansion (see e.g. Edmonds 1957, p. 81)

$$
\exp(i\mathbf{k}\cdot\mathbf{r})=4\pi\sum_{l,m} i^l\,j_l(kr)\,Y_{lm}(\vartheta,\varphi)\,Y^*_{lm}(\theta,\pi)
\tag{3.6}
$$

into the expressions (2.8) for $I_1 \ldots I_7$, and going over to A, E, F and G via (2.7) and (3.3), we obtain after somewhat lengthy calculations, which involve the use of various relations between Legendre and associated Legendre polynomials (see e.g. Edmonds 1957, p. 23), the final formulas

$$
\begin{aligned}
A(\theta) &= 4\pi\sum\{e^{i\eta_l}\,a_l+e^{i\eta_{-l-1}}\,a_{-l-1}\}\,P_l^1(\cos\theta),\\
E(\theta) &= 4\pi\sum\{-e^{i\eta_l}\,(l+1)\,[a_l+(l-1)\,b_l]+e^{i\eta_{-l-1}}\,l\,[a_{-l-1}-(l+2)\,b_{-l-1}]\}\,\frac{P_l^1(\cos\theta)}{l(l+1)},\\
F(\theta) &= 2\pi\sum\{e^{i\eta_l}\,[(l+1)\,a_l+(l-1)\,b_l]-e^{i\eta_{-l-1}}\,[l\,a_{-l-1}+(l+2)\,b_{-l-1}]\}\,P_l(\cos\theta),\\
G(\theta) &= 2\pi\sum\{e^{i\eta_l}\,(l+1)\,[a_l-b_l]+e^{i\eta_{-l-1}}\,l\,[-a_{-l-1}+b_{-l-1}]\}\,\frac{P_l^2(\cos\theta)}{l(l+1)}.
\end{aligned}
\tag{3.7}
$$

a_l and b_l are the following combinations of radial matrix elements, corresponding to absorption of electric and magnetic radiation multipoles:

$$
\begin{aligned}
a_l \quad &= \int g_l\,f_l\,j_{l-1}(kr)\,r^2\,dr+\frac{1}{2l+1}\int f_l\,g_l\,j_{l-1}(kr)\,r^2\,dr-\\
&\qquad -\frac{2l}{2l+1}\int f_l\,g_l\,j_{l+1}(kr)\,r^2\,dr;\quad l=1,2,\ldots
\end{aligned}
$$

$$a_{-l-1} = \int g_i f_{-l-1} j_{l+1}(kr) r^2 dr - \frac{1}{2l+1}\int f_i g_{-l-1} j_{l+1}(kr) r^2 dr - \\ - \frac{2(l+1)}{2l+1}\int f_i g_{-l-1} j_{l-1}(kr) r^2 dr; \quad l = 1, 2, \ldots$$

$$b_l \;= \int [g_i f_l + f_i g_l]\, j_{l-1}(kr) r^2 dr; \quad l = 2, 3, \ldots$$

$$b_{-l-1} = \int [g_i f_{-l-1} + f_i g_{-l-1}]\, j_{l+1}(kr) r^2 dr; \quad l = 0, 1, \ldots \tag{3.8}$$

a_l and a_{-l-1} correspond to electric multipoles of order l. b_l and b_{-l-1} correspond to magnetic multipoles of order $l-1$ and $l+1$, respectively.

For the total cross section we obtain from (1.15), (3.3) and (3.7)

$$\sigma = C' \tfrac{1}{2} \int \{|A|^2 + |B|^2 + |C|^2 + |D|^2\}\, d\Omega = \\ = 32\pi^3 C' \sum_{l=1}^{\infty} \{(l+1) a_l^2 + l a_{-l-1}^2 + l b_{l+1}^2 + (l+1) b_{-l}^2\}. \tag{3.9}$$

The quantities a_0 and b_0 that occur formally in $F(\theta)$ in (3.7) should be put equal to zero.

The expansions (3.7) can, of course, also be obtained directly from (1.4), inserting for $\hat{\mathbf{e}} \exp(i\,\mathbf{k}\cdot\mathbf{r})$ an expansion in electric and magnetic multipoles, and for ψ_f the partial waves expansion. Although one then has to make the spin analysis again, this method may have the advantage of leading more directly to the form (3.2), and also of giving automatically the special combinations a_l and b_l in (3.7). In the method used here this special choice comes in more indirectly, e.g. from the requirement that the total cross section (3.9) should not contain any cross products.

4. An approximate final state wave function in a Coulomb field

We now assume the electron to move in a Coulomb potential

$$V(r) = -a/r, \quad a = \alpha Z, \quad \alpha = e^2/\hbar c, \tag{4.1}$$

and will derive expressions for the reaction amplitudes to relative order a. This means, as will be seen, that we must have expressions for ψ_i and ψ_f to order a^2.

For the initial $1\,S_{\frac{1}{2}}$-state (K-shell state) we have (see e.g. Bethe and Salpeter 1957, p. 155)

$$g_i = N_i r^{\gamma-1} e^{-ar}, \quad f_i = -\left(\frac{1-\gamma}{1+\gamma}\right)^{\frac{1}{2}} g_i, \tag{4.2}$$

where $\gamma = \sqrt{1-a^2}$ is the corresponding eigenvalue of ε; $1-\gamma$ is the binding energy of the K-shell. The normalization constant N_i is

$$N_i = \left(\frac{(1+\gamma)(2a)^{2\gamma+1}}{8\pi\Gamma(2\gamma+1)}\right)^{\frac{1}{2}} = \frac{a^{3/2}}{\pi^{\frac{1}{2}}}[1 + 0(a^2 \ln a)]. \tag{4.3}$$

In the relevant approximation we can put

$$\left(\frac{1-\gamma}{1+\gamma}\right)^{\frac{1}{2}}=\tfrac{1}{2}\,a. \tag{4.4}$$

Looking at ψ_f, we see from the fact that the zeroth order approximation is a plane wave, that f_+ and f_- in (2.5) start as a^0, whereas g_+ and g_- are of order a. Inspection of (2.8) shows that, apart from the normalization constant N_i, all integrals are of order a; I_6, which seems to form an exception, really also starts as a, as is easily seen by using $f_-\sim e^{ipz}$, $g_i\sim e^{-ar}$ and performing the integration.

To obtain expressions for $I_1 \dots I_7$ to relative order a, we must then have f_+ and g_+ to order a and f_- and g_- to order a^2. The exponent $\gamma-1$ in (4.2) can be equated to zero everywhere except in I_6.

The desired second-order final state wave function can be obtained by a second-order Born approximation; this is the method used by Gavrila 1959 in his derivation of the differential cross section to relative order a. Due to the infinite range of the Coulomb potential, one must apply the Born approximation to the Yukawa potential $e^{-\lambda r}/r$, and afterwards let $\lambda\to 0$. In this limit there appear (in second order) divergences in the matrix elements; however, as shown by Gavrila, these divergences cancel in the expression for the cross section.

We shall use a different method, consisting of an improvement of the approximate Sommerfeld-Maue wave function. This wave function was used by Sommerfeld 1939 for a derivation of the lowest order (Sauter) approximation of the differential cross section. The infinite range of the Coulomb potential is taken into account exactly, and no infinities occur when we improve the wave function to take the potential into account to second order. In addition the lowest order expressions for the reaction amplitudes will be valid for all $\beta=v/c$, thus giving a smooth transition to the non-relativistic results. The Born approximation is valid only for $a\ll\beta$, being actually an expansion in a/β.

To derive our approximation for ψ_f we go over to the second-order Dirac equation by applying the operator $i\boldsymbol{\alpha}\cdot\mathrm{grad}-\alpha_m+V-\varepsilon$ on the Dirac equation (2.1); the result is

$$[\Delta+p^2-2\varepsilon V+V^2+i(\boldsymbol{\alpha}\cdot\mathrm{grad}\,V)]\,\psi=0. \tag{4.5}$$

We are interested in the incoming scattering solution of (4.5), i.e. the solution with asymptotic form (1.3). As every solution of the first-order Dirac equation is also a solution of (4.5), it follows from the uniqueness of the scattering solutions that a solution of (4.5) and (1.3) is also a solution of (2.1), provided the asymptotic plane wave spinor $\exp(i\,\mathbf{p}\cdot\mathbf{r})\,w$ in (1.3) is a solution of the free Dirac equation, i.e., with suitable normalization,

$$w=\left(\frac{\varepsilon+1}{2\varepsilon}\right)^{\frac{1}{2}}\left(v_+ +\frac{p}{\varepsilon+1}\,\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\,v_-\right)u. \tag{4.6}$$

(See Nagel 1960 for a more extensive discussion of this point.)

The Sommerfeld-Maue wave function (Sommerfeld and Maue 1935; Sommerfeld

1939, and Bethe and Maximon 1954) is a solution of (4.5) to first order in V, and has the form

$$\psi_1 = e^{ipz}\left(1 - \frac{i}{2\varepsilon}\boldsymbol{\alpha}\cdot\operatorname{grad}\right) F w, \tag{4-7}$$

where $e^{ipz} F$ is the solution of

$$(\Delta + p^2 - 2\varepsilon V)\,\psi = 0 \tag{4.8}$$

with asymptotic form e^{ipz} + inc. spher. wave.

If we put $\psi = \psi_1 + \psi_2$, where ψ is the exact solution of (4.5), we get from (4.5) and (4.7) the following inhomogeneous equation for ψ_2:

$$[\Delta + p^2 - 2\varepsilon V + V^2 + i(\boldsymbol{\alpha}\cdot\operatorname{grad} V)]\,\psi_2 = \\ - e^{ipz}\left[V^2\left(1 - \frac{i}{2\varepsilon}\boldsymbol{\alpha}\cdot\operatorname{grad}\right) + \frac{1}{2\varepsilon}(\boldsymbol{\alpha}\cdot\operatorname{grad} V)\,\boldsymbol{\alpha}\cdot\operatorname{grad}\right] F w, \tag{4.9}$$

and boundary condition: incoming spherical wave.

We get the V^2 order part of ψ_2 by solving (4.9) after dropping all terms in V on the left hand side and keeping only V^2 terms on the right hand side; this gives

$$\psi_2 = \frac{1}{4\pi}\int \frac{\exp(-ip|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\, e^{ipz'}\left[V^2 F_0 + \frac{1}{2\varepsilon}(\boldsymbol{\sigma}\cdot\operatorname{grad}' V)\,(\boldsymbol{\sigma}\cdot\operatorname{grad}' F)_1\right] d\mathbf{r}'\, w. \tag{4.10}$$

F_0 and $(\operatorname{grad} F)_1$ means that we shall take only the lowest (zeroth and first) order term of F and $\operatorname{grad} F$, respectively.

For $V = -a/r$ the relevant F is

$$e^{\frac{1}{2}\pi\varkappa}\,\Gamma(1 + i\varkappa)\ {}_1F_1(-i\varkappa;\ 1;\ -ip(r+z)), \tag{4.11}$$

where ${}_1F_1$ is the confluent hypergeometric function.

Combining (4.7) and (4.10), with F as given by (4.11) and w as in (4.6) $(\hat{\mathbf{p}} = \hat{\mathbf{z}})$, and using

$$(\operatorname{grad}\,{}_1F_1)_1 = -ip(\hat{\mathbf{r}} + \hat{\mathbf{z}})\,\varkappa\,\frac{\exp(-ip(r+z)) - 1}{p(r+z)}, \tag{4.12}$$

we get by comparison with (2.5) the following expressions for f_+^* etc. to the necessary orders in a:

$$f_+^* = N_f\left\{e^{-ipz}\,{}_1F_1(i\varkappa;\ 1;\ ip(r+z)) - a\,\frac{p}{2(\varepsilon+1)}\,e^{-ipz}\,\frac{\exp[ip(r+z)] - 1}{pr}\right\},$$

$$g_+^* = N_f\left\{-a\,\frac{p}{2(\varepsilon+1)}\,e^{-ipz}\,\frac{\exp[ip(r+z)] - 1}{pr}\,\frac{\sin\vartheta}{1+\cos\vartheta}\right\},$$

$$f_-^* = N_f\left\{\frac{\mathbf{p}}{\varepsilon+1}\,e^{-ipz}\,{}_1F_1(i\varkappa;\ 1;\ ip(r+z)) - a\,\frac{e^{-ipz}}{2\varkappa}\,{}_1F_1'(i\varkappa;\ 1;\ ip(r+z))\,(1+\cos\vartheta)\right. \\ \left. + a^2\,\frac{p}{4\pi(\varepsilon+1)}\int \frac{\exp(ip|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\,\frac{e^{-ipz'}}{r'^2}\left(1 + \frac{i}{2}\,\frac{\exp[ip(r'+z')] - 1}{pr'}\right) d\mathbf{r}'\right\},$$

$$g_-^* = N_f\left\{-a\frac{e^{-ipz}}{2\varkappa}\,{}_1F_1'(i\varkappa;\,1;\,ip(r+z))\sin\vartheta + \right.$$

$$\left. + i a^2 \frac{p}{8\pi(\varepsilon+1)}\int \frac{\exp(ip|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}\,\frac{e^{-ipz'}}{r'^2}\,\frac{\exp[ip(r'+z')]-1}{pr'}\,\frac{\sin\vartheta'\cos(\varphi'-\varphi)}{1+\cos\vartheta'}\,d\mathbf{r}'\right\}. \tag{4.13}$$

Here

$$N_f = \left(\frac{\varepsilon+1}{2\varepsilon}\right)^{\frac{1}{2}} e^{\frac{1}{2}\pi\varkappa}\,\Gamma(1-i\varkappa). \tag{4.14}$$

It should be observed that in (4.13) the terms containing the ${}_1F_1$-function (or its derivative) are correct for all $\varkappa = a/\beta$, whereas the other terms, which give contributions of relative order a in the matrix elements, are valid under the assumption $\varkappa \ll 1$; only then is (4.10) a good approximation, and it is then meaningless to give a more accurate form for the other terms giving contributions of relative order a.

The factor $\sin\vartheta'\cos(\varphi'-\varphi)$ in the integral for g_-^* may require a comment: from (4.10) one obtains $\sigma_{\varphi'}\sin\vartheta'$, which is rewritten, using

$$\sigma_{\varphi'} = \boldsymbol{\sigma}\cdot\hat{\boldsymbol{\varphi}}' = \boldsymbol{\sigma}\cdot[\cos(\varphi - \varphi)\,\hat{\boldsymbol{\varphi}} + \sin(\varphi'-\varphi)\,\hat{\mathbf{z}}\times\hat{\boldsymbol{\varphi}}].$$

The second term gives zero when we integrate over $\mathbf{r}'$.

5. The reaction amplitudes to relative order αZ

Inserting (4.2) and (4.13) into the integrals in (2.8) we get a number of rather complicated three-dimensional integrals. The evaluation of these integrals, which can all be expressed in elementary functions, is performed in the Appendix. We give here the resulting expressions for A, B, C and D in the form

$$A(\theta) = K\{A_0(\theta) + a[A_{1R}(\theta) + i A_{1I}(\theta)] + 0(a^2)\}\ \text{etc.}, \tag{5.1}$$

where A_0, A_{1R} and A_{1I} are real functions, and K is a factor common to A, B, C and D. The expressions for A_{1R}, A_{1I} etc. have been obtained under the assumption $a \ll \beta$; this fact has been used when we extract the factor K also from these terms.

For shortness we introduce auxiliary functions X, Y, Z, U and V:

$$\left.\begin{aligned}
X &= 2\varepsilon k(1-\beta\cos\theta) \approx 2\varepsilon(\varepsilon-1)(1-\beta\cos\theta),\ [\text{as } k = \varepsilon - \sqrt{1-a^2}]\\
Y &= \frac{p}{\varepsilon-1} - \cos\theta,\\
Z &= \frac{\ln\varepsilon(1-\beta\cos\theta) + \cos\theta\ln\varepsilon(1+\beta)}{(\varepsilon-1)p^2\sin^2\theta},\\
U &= \frac{X^{\frac{1}{2}} - (\varepsilon-1)Y}{(\varepsilon-1)p^2\sin^2\theta},\\
V &= \frac{2}{X} - \frac{\ln\varepsilon(1+\beta)}{p(\varepsilon-1)}.
\end{aligned}\right\} \tag{5.2}$$

The results are then

$$\left.\begin{aligned} A_0 &= 4\pi \frac{p}{\varepsilon+1} \frac{\sin\theta}{X^2} [2(\varepsilon+3)-X], \\ B_0 &= -4\pi\, 2(\varepsilon-1)^2 \frac{\sin^2\theta}{X^2}, \\ C_0 &= 4\pi\, 2p(\varepsilon-1) \frac{\sin^2\theta}{X^2}, \\ D_0 &= 4\pi \frac{\sin\theta}{X^2} [X-2(\varepsilon-1)]. \end{aligned}\right\} \tag{5.3}$$

$$\left.\begin{aligned} A_{1R} &= \pi^2 \sin\theta \left[\frac{4p}{\varepsilon+1} \frac{1}{X^{\frac{3}{2}}} - \frac{2}{p} \frac{1}{X^{\frac{1}{2}}} + \cos\theta\, U + \frac{1}{p^2}\right], \\ B_{1R} &= \pi^2 \left[2\frac{\varepsilon-1}{\varepsilon+1} \frac{1}{X^{\frac{3}{2}}} - \frac{2\varepsilon}{p^2} \frac{1}{X^{\frac{1}{2}}} + \frac{2\cos\theta}{X^{\frac{1}{2}}} U + \frac{1}{p(\varepsilon-1)}\right], \\ C_{1R} &= \pi^2 \left[-\frac{2p}{\varepsilon+1} \frac{1}{X^{\frac{3}{2}}} + \frac{2}{p} \frac{1}{X^{\frac{1}{2}}} + \frac{2U}{X^{\frac{1}{2}}} - \frac{1}{p^2}\right], \\ D_{1R} &= \pi^2 \sin\theta\, U. \end{aligned}\right\} \tag{5.4}$$

$$\left.\begin{aligned} A_{1I} &= -\pi \sin\theta\, [V + (\varepsilon-1-p\cos\theta) Z], \\ B_{1I} &= -\pi \left[\left(\frac{\varepsilon-3}{p} + \cos\theta\right) V + (2\cos\theta + p\sin^2\theta) Z\right], \\ C_{1I} &= \pi \left[\left(1 + \frac{p}{\varepsilon+1} \cos\theta\right) V - (2-(\varepsilon-1)\sin^2\theta) Z\right], \\ D_{1I} &= \pi \sin\theta \left[\frac{p}{\varepsilon+1} V + (\varepsilon-1) Y Z\right]. \end{aligned}\right\} \tag{5.5}$$

For K we have

$$K = \tfrac{1}{2} a N_i N_f (1 - i\varkappa) e^{i\delta} e^{i\varkappa \ln(1-\beta\cos\theta)} \exp\left(-\varkappa \operatorname{arctg} \frac{\varkappa(\varepsilon+1)}{\varkappa^2-\varepsilon}\right). \tag{5.6}$$

Here δ is an angle-independent phase-factor, which goes to zero as $\beta \to 0$; the value of arctg should be chosen in $(0, \pi)$.

The lowest order terms (5.3), which correspond to the Sauter approximation, are rather simple, and give reasonably short expressions for the cross sections and polarizations. The first-order correction terms (5.4) and (5.5) are much more complicated, and we will not give the corresponding analytic expressions for the observable quantities. The expression for the first-order correction to the differential cross section, involving products of zeroth and first order real terms, has been given by Gavrila 1959. Our relative differential cross section should agree with Gavrila's; we have not checked this directly, but, as will be seen later on, the expressions for the integrated cross section are the same.

To get an idea of the influence of the first-order terms A_{1R} etc. on the cross sections and polarizations, we have computed numerically the functions $A_0(\theta) \ldots D_{1I}(\theta)$ for three energies, $\varepsilon = 1.5$, 2 and 3 ($\beta = 0.745$, 0.866, and 0.943), i.e. photoelectron energies of about 0.25, 0.5 and 1 MeV. The results are discussed in the next section.

For small β, A_0 is the dominating term; B_0, C_0 and D_0 are of relative order β^2 at least. Even the first-order terms are of order β (or higher) compared to A_0. As has been pointed out earlier, the expressions for the first-order terms are unreliable when $\beta \leqslant a$, but an exact investigation, using the expansions in Sect. 3, of the limit $\beta \to 0$ shows that the corrections of order a actually vanish in this limit, so that for $\beta = 0$ the relativistic corrections are of order a^2 and higher (see Nagel and Olsson 1960).

6. Results and discussion

a. *Angular distribution, unpolarized photons*

Although the angular distribution (including the case of linearly polarized photons) to relative order a has been given by Gavrila, we shall give a discussion here, as the formula in Gavrila's paper is rather complicated.

The relative angular distribution is (see (1.15))

$$\sigma(\theta) \sim I_0(\theta) + a I_1(\theta) + \cdots, \tag{6.1}$$

where
$$I_0 = A_0^2 + B_0^2 + C_0^2 + D_0^2 = \\ = 32\,\pi^2 \frac{1}{\varepsilon^4(\varepsilon-1)^3} \frac{\sin^2\theta}{(1-\beta\cos\theta)^4}\left[1 + \frac{\varepsilon(\varepsilon-1)(\varepsilon-2)}{2}(1-\beta\cos\theta)\right] \tag{6.2}$$

s the Sauter cross section, and

$$I_1 = 2(A_0 A_{1R} + B_0 B_{1R} + C_0 C_{1R} + D_0 D_{1R}). \tag{6.3}$$

In (6.2) we have put $k = \varepsilon - 1$, cf. (5.2).

Graphs of I_0 and I_1 for $\varepsilon = 2$ are given in Fig. 2, p. 21. For $\varepsilon = 1.5$ and 3 similar curves are obtained, except that the relative importance of I_1 is smaller for $\varepsilon = 3$ than for 1.5 and 2; see Fig. 7, p. 22, for the ratio of the integrated cross sections I_1 and I_0. It is seen from Fig. 2 that the influence of I_1 on the relative cross section is very small, both because I_1 is considerably smaller than I_0, and because I_1 has about the same angular dependence as I_0. There is a slight tendency of I_1 to push the angle $\theta_{\max}$ of maximum emission towards larger angles and to increase the emission for angles larger than $\theta_{\max}$. Both these features are present in the experimental angular distributions obtained by Hultberg 1959, but especially the emission for large angles, obtained in the experiments, is much larger than can be explained even qualitatively by the first-order correction I_1. For heavy atoms—Hultberg's results refer to $Z = 92$—the higher order corrections in a must be expected to be at least as important as the first-order correction.

From (6.3) and the fact (see (5.3)) that A_0, B_0, C_0 and D_0 vanish for $\theta=0$ and π, it follows that the forward and backward intensities must be zero even in first order (cf. Gavrila 1960). The forward (and backward) intensity is of order a^2, and the a^2 order term is evidently obtained in the form (cf. (1.7))

$$I(0)=a^2\,2\,(B_{1R}^2+B_{1I}^2). \tag{6.4}$$

In Fig. 3, p. 21, we show the resulting ratio

$$\varkappa_0=I(0)/I_0(\theta_{\max}) \text{ (in units } a^2) \tag{6.5}$$

of forward to maximum emission, as function of energy. The figure also shows the three experimental points obtained by Hultberg for $Z=92$. The theoretical and experimental ratios show the same tendency to increase with energy, but the quantitative agreement is bad; again, this should not be surprising, in view of the importance of higher order terms for such large Z-values. Banerjee's conjecture (Banerjee 1958) that $\varkappa_0$ should decrease as the energy increases was based on the incorrect assumption that the finite forward intensity should be of order a/ε. Sauter and Wüster 1955 have performed a numerical calculation of $\varkappa_0$ for $h\nu=1332$ keV and $Z=82$, obtaining the value 0.27 in rather good agreement with the experimental 0.245 (for $Z=92$). They also give an approximate value 0.21; this value was computed taking into account only a part of the first-order corrections in the matrix elements, which explains the disagreement with our result (~ 0.42).

We also obtain in order a^2 a non-zero value for $I(\pi)/I_0(\theta_{\max})$, but this ratio is very small, 0.007 a^2 for $\varepsilon=1.5$, and decreasing rapidly as the energy increases.

It is possible that the vanishing in lowest order of B and C for $\theta=0$ and π is accidental for the Coulomb potential. If we use a screened potential we might then get a finite forward intensity even in lowest order. This could be so only for relativistic energies, because non-relativistically, when spin effects are ignored, B, C and D must vanish identically (cf. (1.6)).

b. *Angular distribution, linearly polarized photons*

This distribution is obtained from (1.14). If we take the lowest order (Sauter) approximation, for $\varepsilon=1$ (low-energy limit) no emission takes place perpendicular to the polarization plane, but as the energy increases, part of the electrons are emitted also in the perpendicular plane, until for $\varepsilon\gg 1$ the distribution is independent of the azimuthal angle ϕ. The effect of the terms of first order in a is rather small; in the energy range $\varepsilon=3$ to 5 they increase somewhat, by a factor $1+0.3\,a$, the ratio of emission in and perpendicular to the polarization plane. The behaviour for $\varepsilon=1$ and for $\varepsilon=\infty$ is not changed.

If one studies the asymmetry ratio for a fixed θ, say $\pi/2$, there even occurs, in the Sauter approximation, a "crossover", so that for $\varepsilon>2$ the emission in the polarization plane is smaller than in the perpendicular plane (see graph in McMaster and Hereford 1954). The effect of the a-order correction is to diminish this ratio, by a factor which is about $1-a$ in the region $\varepsilon=1.5$ to 3, thus causing the crossover to occur at a somewhat lower energy than $\varepsilon=2$.

The experimental results on this point are somewhat contradictory. McMaster and Hereford, loc. cit., using Compton-scattered photons to produce photoelectrons from Pb, found the crossover to occur in fair agreement with the Sauter results, whereas Brini et al. 1957, using an experimental arrangement, which should enable them to count only the K-shell photoelectrons from Pb, found the ratio to be larger than one everywhere in the interesting energy region.

c. *Electron polarization*

We shall study only the polarizations P_1, P_2 and P_3, (1.17)–(1.20), obtained from circularly polarized or unpolarized photons. Let us first remark that from the relations (1.7) and (1.8) it follows, if $B(0)$ and $B(\pi)$ are different from zero, that $P_1 = P_3 = 0$ for $\theta = 0$ and π, and $P_2(0) = 1$, $P_2(\pi) = -1$. However, in the approximate expressions studied below, these relations may not be fulfilled, as a consequence of the vanishing of B_0 (and C_0) in the forward and backward directions.

In the limit $\beta \to 0$ all polarization effects vanish in the approximation considered here. However, the higher orders in a give non-vanishing and for heavy atoms even considerable polarization effects also at the K-shell threshold, as will be seen in a following paper (Nagel and Olsson 1960).

P_1, the transverse polarization perpendicular to the scattering plane, is a first-order effect in a, and is given in this order by

$$P_1 = a\,\frac{2\left[-A_0 B_{1I} + A_{1I} B_0 - C_0 D_{1I} + C_{1I} D_0\right]}{A_0^2 + B_0^2 + C_0^2 + D_0^2}. \tag{6.6}$$

Graphs of P_1/a as function of θ for the three energies are given in Fig. 4, p. 21. P_1 is, for these energies, fairly constant over the angular region where most of the photoelectrons are emitted. P_1 is a polarization analogous to that obtained in relativistic Coulomb scattering of unpolarized electrons, and can be studied experimentally in the same way by observing the left-right asymmetry in Coulomb scattering of the outgoing electrons. The transverse polarization in electron scattering vanishes as ε^{-1} for large ε; as will be seen in (*e*) in this section, P_1 also behaves, at least in first order in a for the photoelectrons going out in the peak of maximum emission, as ε^{-1}, so that it must attain a maximum for some energy larger than $\varepsilon = 2$. The higher orders in a give a P_1 different from zero even in the limit $\beta = 0$.

The longitudinal and transverse polarizations P_2 and P_3 in the scattering plane, obtained with circularly polarized photons, are different from zero even in the lowest order approximation:

$$P_2 = \frac{p}{\varepsilon + 1}\,\frac{1 + \frac{1}{2}\varepsilon(\varepsilon^2 - 2\varepsilon - 1)(1 - \beta\cos\theta)}{1 + \frac{1}{2}\varepsilon(\varepsilon - 1)(\varepsilon - 2)(1 - \beta\cos\theta)} \tag{6.7}$$

$$P_3 = (\varepsilon - 1)\,\frac{\sin\theta}{1 + \frac{1}{2}\varepsilon(\varepsilon - 1)(\varepsilon - 2)(1 - \beta\cos\theta)}. \tag{6.8}$$

In Figs. 5 and 6, p. 22, we give graphs of P_2 and P_3, as obtained from (6.7) and (6.8), and also of the first-order corrections $f(\theta)$, defined by

$$P_{\mathrm{corr}} = [1 + a\, f(\theta)]\, P. \tag{6.9}$$

For the longitudinal polarization P_2 the effect of $f(\theta)$ is to diminish the polarization by about $1 - 0.3\,a$ in the angular region of greatest interest, for these energies.

The correct lowest order expressions for the electron polarizations corresponding to circular photon polarization were first given by Olsen 1958. Banerjee (1958, 1959), using the Sommerfeld-Maue wave function, arrived independently at these results, and also gave those corrections of order a that survive in the limit $\varepsilon \to \infty$. In a paper by Fano, McVoy and Albers 1959 there is a very extensive and illuminating discussion, with many graphs, of these lowest order polarizations.

To our knowledge no experimental investigations on electron polarizations in the photoeffect have been published.

d. *Total cross section*

The total cross section (per K-electron) is obtained by integration of (1.15), and can be written in the form

$$\sigma = T\, \sigma_S\, (1 + a\, f(\varepsilon) + \cdots), \tag{6.10}$$

with

$$T = \frac{2\pi\varkappa\,(1+\varkappa^2)}{1 - e^{-2\pi\varkappa}} \exp\left[-2\varkappa \operatorname{arctg} \frac{\varkappa(\varepsilon+1)}{\varkappa^2 - \varepsilon}\right], \text{ cf. (5.6).} \tag{6.11}$$

σ_S is the Sauter cross section

$$\sigma_S = \frac{8\pi}{3}\left(\frac{\hbar}{m c}\right)^2 \alpha^6 Z^5 \left(\frac{m c^2}{h \nu}\right)^5 p^3 N_0(\varepsilon). \tag{6.12}$$

$$f(\varepsilon) = \frac{\int I_1(\theta)\, d\Omega}{\int I_0(\theta)\, d\Omega} = \frac{N_1(\varepsilon)}{N_0(\varepsilon)} \tag{6.13}$$

with

$$N_0(\varepsilon) = 1 + \frac{3\varepsilon(\varepsilon-2)}{4(\varepsilon+1)}\left\{1 - \frac{1}{2\beta\varepsilon^2} \ln \frac{1+\beta}{1-\beta}\right\}, \tag{6.14}$$

$$N_1(\varepsilon) = \frac{3\pi}{4} \frac{p}{(\varepsilon+1)^2}\left[\frac{-19\varepsilon^2 + 41\varepsilon + 8}{15} + \frac{\varepsilon^2(\varepsilon-2)}{(\varepsilon-1)}\left\{1 - \frac{1}{2\beta\varepsilon^2} \ln \frac{1+\beta}{1-\beta}\right\}\right]. \tag{6.15}$$

In the derivation of (6.10) we have used, in the dominant term for small β, the exact expression for X in (5.2); this gives four of the five powers of $m c^2/h \nu$ in (6.12).

The formula for σ agrees with that obtained by Gavrila 1959, if we expand T to first order in $\varkappa$. For small β, $T\,\sigma_S$ goes over into the non-relativistic Stobbe cross section (see e.g. Bethe and Salpeter 1957, p. 390). $f(\varepsilon)$ goes to zero with β; this is strictly true, even if the form given above for $f(\varepsilon)$ is not reliable when

$\beta \leqslant a$. A graph of $f(\varepsilon)$ as function of ε is given in Fig. 7, p. 22. The behaviour of $f(\varepsilon)$ for small β, and for large ε is:

$$\beta \ll 1, \; f(\varepsilon) = \frac{\pi}{8}\beta\,(1 + \beta^2/2 + \cdots), \tag{6.16}$$

$$\varepsilon \gg 1, \; f(\varepsilon) = -\frac{4\pi}{15}\left(1 - \frac{41}{6\varepsilon} + \cdots\right). \tag{6.17}$$

For large ε, $f(\varepsilon)$ goes to $-4\pi/15 = -0.838$. This limit is, however, approached very slowly, as is seen from (6.17) and Fig. 7.

To give an idea of the accuracy of (6.10) we have tabulated (Table 1) the ratio σ/σ_S for three values of Z and three photon energies ($Z = 26$, 50 and 84; $h\nu/mc^2 = 0.693$, 2.212 and ∞), compared with the "exact" values in ( ); for the lower energies these exact values are taken from the numerical calculations of Hulme et al. 1935, for $h\nu/mc^2 = \infty$ from the work of Pratt 1960. The values in [ ] are obtained from an approximate formula proposed by Pratt, which combines the a-dependence of his high-energy limit cross section with the energy dependence given by $f(\varepsilon)$ (from Gavrila's work). This formula should be a good approximation at high energies.

Table 1

$h\nu/mc^2$	$Z=26$	$Z=50$	$Z=84$
0.693	0.59 (0.62) [0.60]	0.45 (0.50) [0.44]	0.44 (0.51) [0.34]
2.212	0.60 (0.63) [0.64]	0.43 (0.51) [0.50]	0.32 (0.47) [0.44]
∞	0.49 (0.53)	0.26 (0.34)	0.11 (0.22)

e. *The high-energy limit*

For large ε the emission of photoelectrons is concentrated in a narrow peak around an angle θ of order ε^{-1}. We will keep only the dominant terms in ε of $A_0 \ldots D_{1l}$ for these θ, and study the resulting expressions. However, it should be stressed, cf. the behaviour of $f(\varepsilon)$ in (d), that these limits can be expected to be approached very slowly.

Put $x = \varepsilon\theta$; then we have e.g. $X = 1 + x^2$ etc. After suitable expansions we get to first order in a:

$$|A|^2 + |B|^2 = |C|^2 + |D|^2 = |K|^2\,(8\pi)^2 \frac{x^2}{(1+x^2)^3}\left[1 - a\frac{\pi}{2}\frac{1}{\sqrt{1+x^2}}\right]. \tag{6.18}$$

This shows, if we compare with (1.14), that to first order in a the distribution is, for these θ-values at least, independent of ϕ in the high-energy limit.

(6.18) attains its maximum

$$|K|^2 (8\pi)^2 \frac{4}{27}\left(1 - a\frac{\pi}{\sqrt{6}}\right) \tag{6.19}$$

for

$$x = \frac{1}{\sqrt{2}}\left(1 + a\frac{\pi}{8\sqrt{6}}\right). \tag{6.20}$$

Thus, even in the high-energy limit we still have the tendency of the first-order correction to increase the angle $\theta_{\max}$, though the correction now subtracts from the Sauter distribution.

For the forward to maximum intensity we find the asymptotic value

$$\varkappa_0 = 5.85\, a^2. \tag{6.21}$$

For the polarizations we obtain, to order a,

$$P_1 = 0\,(a/\varepsilon), \quad P_2 = 1 + 0\,(\varepsilon^{-1}), \quad P_3 = 0\,(\varepsilon^{-1}). \tag{6.22}$$

The high-energy results given here agree, in the relevant cases, with those that can be derived from the formulas given by Banerjee 1959.

7. Conclusions

Some of the effects studied in this paper, as the finite forward emission and the transverse polarization of the photoelectrons, come from the terms of relative order αZ in the matrix elements. For the other effects, which appear already in the lowest order approximation, the corrections obtained here are in general rather small, at least for Z-values ($Z < 30 - 40$, say), where one can hope that the first-order terms give the main part of the corrections. For heavy atoms, on the other hand, the first-order terms can at best be expected to give a qualitative indication of the effect of the corrections. To get reliable results for the higher Z-values one has to use the expansions in Sect. 3. This means that one must compute numerically a large number of radial matrix elements, especially if one is interested in the differential cross section and polarizations; for the total cross section relatively fewer radial matrix elements will be expected to suffice. This numerical computation can probably be carried through with a reasonable amount of work only in the case of a pure Coulomb field; in this case, the formalism and series expansions worked out by Olsson 1959 in a number of papers should be of great value. At the K-shell threshold, where the outgoing photoelectrons have zero kinetic energy, one should expect the series expansions in radial matrix elements to converge rapidly, even for the heaviest atoms. This limiting case is studied in a following paper (Nagel and Olsson 1960).

Even if these exact calculations are carried through, it must be remembered that they assume the photoelectron to move in the field of a bare point-nucleus. Although it is probable that, for not too low energies and Z-values, the influence of screening on the total cross section and the general form of the angular photoelectron distribution is not very large, such effects as certain details of the angular distribution—e.g. the forward intensity—and the polarizations may be more sensitive. Other corrections, as the influence of the finite nuclear size and radiative corrections, are probably much less important than the screening corrections.

ACKNOWLEDGEMENTS

In the first place I want to thank Professor L. Hulthén for facilitating my work in various ways. Dr. S. Hultberg's experimental investigations formed one of the main inspiration sources for this work, and Dr. P. O. M. Olsson has contributed much, both in discussions and by his enthusiasm. My thanks are also due to Dr. U. Fano and Dr. R. H. Pratt for kindly sending me preprints of their papers.

The financial support from Statens Råd för Atomforskning is acknowledged with gratitude.

Royal Institute of Technology, Stockholm, Division of Mathematical Physics.

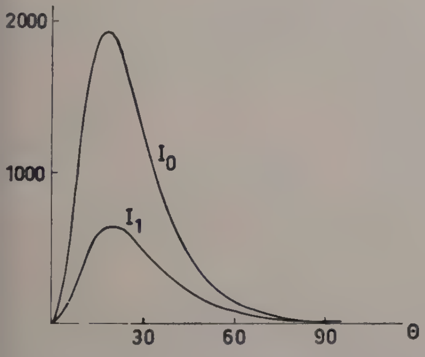

Fig. 2.

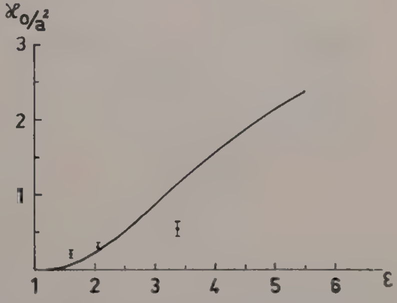

Fig. 3.

Fig. 2. The lowest order (Sauter) angular distribution $I_0(\theta)$ and the first-order correction $I_1(\theta)$, for $\varepsilon = 2$ ($h\nu = 0.5$ MeV). See (6.1).

Fig. 3. The ratio $\varkappa_0$ of forward to maximum intensity, in units a^2, as function of energy. See (6.5). The three experimental points, for $Z = 92$, were obtained by Hultberg 1959.

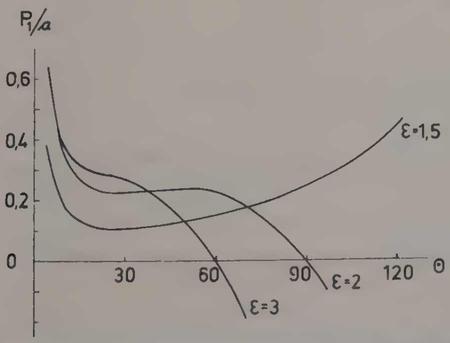

Fig. 4. The transverse electron polarization P_1 (in units a), perpendicular to the scattering plane, as function of θ, for $\varepsilon = 1.5$, 2, and 3. See (6.6).

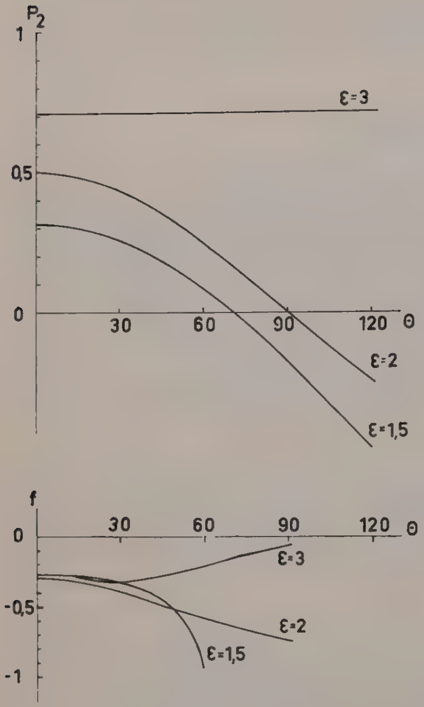

Fig. 5.

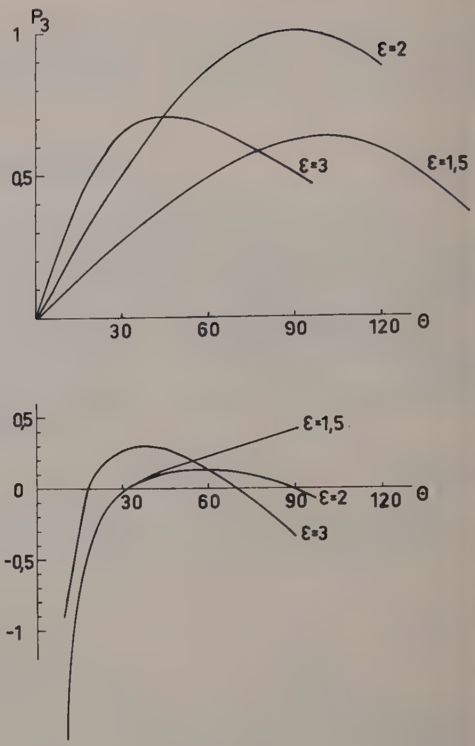

Fig. 6.

Fig. 5. The longitudinal electron polarization P_2, corresponding to circularly polarized photons in lowest order, and the first-order correction $f\ (\theta)$, for three energies. See (6.7) and (6 9).
Fig. 6. The transverse electron polarization P_3 in the scattering plane, corresponding to circularly polarized photons, in lowest order, and the first-order correction $f\ (\theta)$, for three energies. See (6.8) and (6.9).

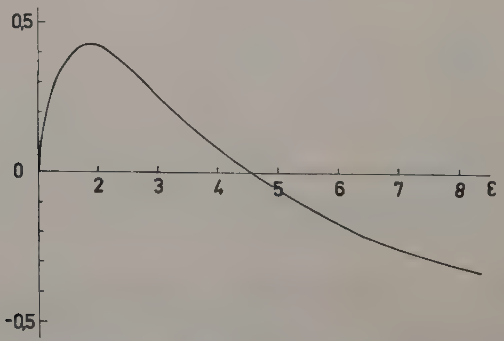

Fig. 7. The ratio $f\ (\varepsilon)$, (6.13), between first and zeroth order total cross sections, as function of energy.

APPENDIX

In this appendix we shall indicate the computation of the integrals $I_1 \dots I_7$, obtained by inserting (4.2) and (4.13) into (2.8).

To save space we use the following abbreviations in (A. 1) and (A. 2): $F = {}_1F_1(i\varkappa;\ 1;\ ip(r+z))$, $H = \exp\,[-ar + i(\mathbf{k}\cdot\mathbf{r} - pz)]$, $J = \{\exp\,[ip(r+z)] - 1\}/pr$. It is convenient to write every integral as a sum of two parts, I^0 and I^1, as follows:

$$\left.\begin{aligned}
I_1^0 &= N i \int H F \cos\vartheta \, d\mathbf{r} \\
I_2^0 &= N i \int H F \sin\vartheta \cos\varphi \, d\mathbf{r} \\
I_3^0 &= I_4^0 = I_5^0 = 0 \\
I_6^0 &= N \frac{1}{\varkappa} \left\{ \frac{2\varepsilon}{\varepsilon+1} \int H F \, d\mathbf{r} - \int H F' (1 + \cos\vartheta) \, d\mathbf{r} \right\} \\
I_7^0 &= N \frac{1}{\varkappa} \int H F' \sin\vartheta \cos\varphi \, d\mathbf{r}
\end{aligned}\right\} \qquad \text{(A. 1)}$$

$$\left.\begin{aligned}
I_1^1 &= -N a \frac{p}{2(\varepsilon+1)} i \int H J \cos\vartheta \, d\mathbf{r} \\
I_2^1 &= -N a \frac{p}{2(\varepsilon+1)} i \int H J \sin\vartheta \cos\varphi \, d\mathbf{r} \\
I_2^1 &= -N a \frac{p}{2(\varepsilon+1)} i \int H J \frac{\sin^2\vartheta \cos 2\varphi}{1 + \cos\vartheta} \, d\mathbf{r} \\
I_4^1 &= -N a \frac{p}{2(\varepsilon+1)} i \int H J \frac{\sin\vartheta \cos\vartheta \cos\varphi}{1 + \cos\vartheta} \, d\mathbf{r} \\
I_5^1 &= -N a \frac{p}{2(\varepsilon+1)} i \int H J \frac{\sin^2\vartheta}{1 + \cos\vartheta} \, d\mathbf{r} \\
I_6^1 &= -N a \frac{p}{2(\varepsilon+1)} \left\{ \frac{4}{a^2} \int (1 - r^{\gamma-1}) H F \, d\mathbf{r} - \right. \\
&\qquad \left. - \frac{1}{\pi} \int\!\!\int \frac{\exp ip|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|} H(\mathbf{r}) \, e^{ip(z-z')} \, r'^{-2} \left(1 + \frac{i}{2} J(\mathbf{r}')\right) d\mathbf{r} \, d\mathbf{r}' \right\} \\
I_7^1 &= -N a \frac{p}{2(\varepsilon+1)} \frac{i}{2\pi} \int\!\!\int \frac{\exp ip|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|} H(\mathbf{r}) \, e^{ip(z-z')} \, r'^{-2} J(\mathbf{r}') \cdot \\
&\qquad\qquad \cdot \frac{\sin\vartheta' \cos\varphi'}{1 + \cos\vartheta'} \, d\mathbf{r} \, d\mathbf{r}',
\end{aligned}\right\} \qquad \text{(A. 2)}$$

Here

$$N = \tfrac{1}{2} a N_i N_f, \qquad \text{(A. 3)}$$

where N_i and N_f are given by (4.3) and (4.14).

As the integrals I^1 give contributions only in the first (relative) order in a, we can, at least in the final results, put $a=0$ in the terms H that occur in (A. 2). The factor $\cos\varphi'$ in the expression for I_7^1 is obtained after some simplification: first one obtains $\cos(\varphi-\varphi')\cos\varphi$; the corresponding integral with $\sin(\varphi-\varphi')\sin\varphi$ evidently has the value zero, as the integrand is an odd function of the variable $\varphi-\varphi'$, so we can add this integral, and hence obtain $\cos\varphi'$.

The integrals I^0, which give the lowest order (Sauter) expressions for the matrix elements, can easily be computed from the integral

$$I(a, \mathbf{q}, \mathbf{p}) = \int \exp(-ar + i\,\mathbf{q}\cdot\mathbf{r})\, r^{-1}\, {}_1F_1(i\varkappa;\, 1;\, i(pr + \mathbf{p}\cdot\mathbf{r}))\, d\mathbf{r} = \frac{4\pi}{a^2+q^2}\left(\frac{a^2+q^2}{a^2+q^2+2\,\mathbf{p}\cdot\mathbf{q} - i\,2\,p\,a}\right)^{i\varkappa}. \tag{A. 4}$$

Here (for a real and >0, $\mathbf{p}$ and $\mathbf{q}$ real, and $p \geqslant 0$) one should use $\arg(a^2+q^2)=0$, and $\arg(a^2+q^2+2\,\mathbf{p}\cdot\mathbf{q}-i\,2\,p\,a)$ in $(-\pi, 0)$.

This integral is given by Sommerfeld 1939, p. 462. It is a special case of an integral computed by Nordsieck 1954; see also Nagel 1960, Appendix A.

With $I(a, \mathbf{q}, \mathbf{p})$ as defined in (A. 4), and

$$\mathbf{q} = \mathbf{k} - \mathbf{p} = |-k\sin\theta,\ 0,\ k\cos\theta - p|,\quad \mathbf{p} = p\,\hat{\mathbf{z}}, \tag{A. 5}$$

we can write (cf. Sommerfeld, loc. cit., p. 487)

$$\begin{aligned} I_1^0 &= N\left[\frac{\partial}{\partial t} I(a, \mathbf{q}+t\,\hat{\mathbf{z}}, \mathbf{p})\right]_{t=0}, \quad I_2^0 = N\left[\frac{\partial}{\partial t} I(a, \mathbf{q}+t\,\hat{\mathbf{x}}, \mathbf{p})\right]_{t=0}, \\ I_6^0 &= N\frac{1}{\varkappa}\left\{-\frac{2\,\varepsilon}{\varepsilon+1}\frac{\partial}{\partial a} I(a, \mathbf{q}, \mathbf{p}) + i\frac{\partial}{\partial p} I(a, \mathbf{q}, p\,\hat{\mathbf{z}})\right\}, \\ I_7^0 &= -N\frac{i}{\varkappa}\left[\frac{\partial}{\partial t} I(a, \mathbf{q}, p\hat{\mathbf{z}} + t\,\hat{\mathbf{x}}\right]_{t=0}. \end{aligned} \tag{A. 6}$$

Performing the operations indicated in (A. 6), we get for the parts of A, B, C and D corresponding to I^0, including first order terms in a:

$$\begin{aligned} A^0(\theta) &= B\sin\theta\,[\varepsilon+3-\varepsilon(\varepsilon-1)(1-\beta\cos\theta)+0(a^2)] \\ B^0(\theta) &= B\,[-p(\varepsilon-1)\sin^2\theta - i\,a\,\varepsilon(\varepsilon-1)(1-\beta\cos\theta)+0(a^2)] \\ C^0(\theta) &= B\,[p^2\sin^2\theta + i\,a\,\varepsilon(\varepsilon-1)\cos\theta\,(1-\beta\cos\theta)+0(a^2)] \\ D^0(\theta) &= B\sin\theta\,[p(\varepsilon-1)-p^2\cos\theta + i\,a\,\varepsilon(\varepsilon-1)(1-\beta\cos\theta)+0(a^2)], \end{aligned} \tag{A. 7}$$

where $$B = 8\pi(1-i\varkappa)\,N\left(\frac{a^2+q^2}{a^2+q^2+2\,p\,\mathbf{q}\cdot\hat{\mathbf{z}} - i\,2\,pa}\right)^{i\varkappa}\frac{1}{(a^2+q^2)^2}\,\frac{p}{\varepsilon+1}. \tag{A. 8}$$

For the expressions in (A. 8) we have

$$X \equiv a^2+q^2 = 2\,k\,\varepsilon\,(1-\beta\cos\theta), \tag{A.9}$$

$$\frac{a^2+q^2}{a^2+q^2+2\,p\,\mathbf{q}\cdot\hat{\mathbf{z}}-i\,2\,pa}=-\,\varepsilon^2\,\frac{\sqrt{1-a^2}-i\,\varkappa}{\varepsilon+i\,\varkappa}\,(1-\beta\cos\theta). \tag{A. 10}$$

(A. 10) gives via (A. 8), and ignoring order a^2, the three last factors in (5.6).

The computation of the integrals $I_1^1 \ldots I_7^1$ in (A. 2) is more complicated. We start with I_1^1 and I_2^1.

Integrating

$$\int \exp\,[-\mu\,r+i\,\mathbf{q}\cdot\mathbf{r}]\,r^{-1}\,d\,\mathbf{r}=4\,\pi\,(\mu^2+q^2)^{-1}\,(\mathrm{Re}\,\mu>0) \tag{A. 11}$$

with respect to μ, we obtain

$$\int \exp\,[-\mu\,r+i\,\mathbf{q}\cdot\mathbf{r}]\,r^{-2}\,d\,\mathbf{r}=\frac{4\pi}{q}\,\mathrm{arctg}\;q/\mu=\frac{2\pi i}{q}\ln\frac{i\,\mu+q}{i\,\mu-q}. \tag{A. 12}$$

Applying twice, with $\mu=a$ and $\mu=a-i\,p$, the trick used to derive I_1^0 and I_2^0 in (A. 6), we have

$$\begin{aligned}\lim_{a\to 0}\int \exp\,[-a\,r+i\,(\mathbf{k}\cdot\mathbf{r}-p\,z)]\,\frac{\exp\,[i\,p\,(r+z)]-1}{p\,r}\,\hat{\mathbf{e}}\cdot\hat{\mathbf{r}}\,d\,\mathbf{r}=&\\ =\frac{2\pi i}{p}\left\{-\frac{\pi}{q^3}\,\hat{\mathbf{e}}\cdot\mathbf{q}+\frac{i}{k^3}\left[\ln\frac{p+k}{p-k}-\frac{2\,p\,k}{p^2-k^2}\right]\hat{\mathbf{e}}\cdot\mathbf{k}\right\},\quad \mathbf{q}=\mathbf{k}-p\,\hat{\mathbf{z}}\,.&\end{aligned} \tag{A. 13}$$

(A. 13) gives

$$I_1^1=N\,a\left[\pi^2\frac{\varepsilon-1}{\varepsilon+1}\,\frac{Y}{X^{\frac{3}{2}}}-i\,\pi\,R\cos\theta\right], \tag{A. 14}$$

$$I_2^1=N\,a\sin\theta\left[\pi^2\frac{\varepsilon-1}{\varepsilon+1}\,\frac{1}{X^{\frac{3}{2}}}+i\,\pi\,R\right], \tag{A. 15}$$

where X and Y are given in (5.2), and $R=\dfrac{p-\ln\varepsilon\,(1+\beta)}{p^2\,(\varepsilon-1)}$.

Postponing I_3^1 till later, we turn to I_4^1 and I_5^1. In I_4^1 we decompose

$$\frac{\sin\vartheta\cos\vartheta\cos\varphi}{1+\cos\vartheta}=\sin\vartheta\cos\varphi-\frac{\sin\vartheta\cos\varphi}{1+\cos\vartheta}.$$

The first term gives I_2^1, while the integral over the second term is equal to

$$\lim_{\varkappa\to 0}\frac{p}{i\,\varkappa}\left[\frac{\partial}{\partial t}\,I\,(a,\,\mathbf{q},\,p\,\hat{\mathbf{z}}+t\,\hat{\mathbf{x}})\right]_{t=0}=-\,4\,\pi\,p\,\frac{\sin\theta}{X}, \tag{A. 16}$$

as is seen from the relation

$${}_1F_1'\,(i\,\varkappa;\,1;\,i\,p\,(r+z))=\varkappa\,\frac{\exp\,[i\,p\,(r+z)]-1}{p\,(r+z)}+0\,(\varkappa^2). \tag{A. 17}$$

Then we get

$$I_4^1 = N a \sin\theta \left[\pi^2 \frac{\varepsilon-1}{\varepsilon+1} \frac{1}{X^{\frac{3}{2}}} + i\pi \left(R - \frac{2p}{\varepsilon+1} \frac{1}{X}\right)\right]. \tag{A. 18}$$

To compute I_5^1 we observe $\dfrac{\sin^2\vartheta}{1+\cos\vartheta} = 1-\cos\vartheta$. The second term is I_1^1, while the first term is seen to give

$$\lim_{\varkappa\to 0} \frac{p}{i\varkappa} \frac{\partial}{\partial p} I(a, \mathfrak{q}, p\,\hat{\mathfrak{z}}) = -4\pi p \frac{Y}{X}. \tag{A. 19}$$

Hence
$$I_5^1 = N a \left[-\pi^2 \frac{\varepsilon-1}{\varepsilon+1} \frac{Y}{X^{\frac{3}{2}}} + i\pi \left(R\cos\theta + \frac{2p}{\varepsilon+1} \frac{Y}{X}\right)\right]. \tag{A. 20}$$

We shall now compute I_3^1, and start from

$$\sin^2\vartheta \cos 2\varphi = \sin^2\vartheta - 2(\sin\vartheta \sin\varphi)^2.$$

The first term gives I_5^1; for the integral over the second term we obtain (observe that $\mathfrak{q}\cdot\hat{\mathfrak{y}} = 0$)

$$\begin{aligned} \int \exp(i\,\mathfrak{q}\cdot\mathfrak{r}) \frac{\exp[i p (r+z)] - 1}{r(1+\cos\vartheta)} (\hat{\mathfrak{y}}\cdot\hat{\mathfrak{r}})^2 d\,\mathfrak{r} &= \\ = -\int_0^\infty da \left\{\lim_{\varkappa\to 0} \frac{p}{\varkappa} \left[\frac{\partial^2}{\partial s\,\partial t} I(a, \mathfrak{q}+s\,\hat{\mathfrak{y}}, p\,\hat{\mathfrak{z}} + t\,\hat{\mathfrak{y}})\right]_{s=t=0}\right\} &= \\ = i\,8\pi p \int_0^\infty \frac{da}{(a^2+q^2)\left[(a-ip)^2 + (\mathfrak{q}+\mathfrak{p})^2\right]} &= \\ = -4\pi \frac{1}{k^2-k_z^2} \left[\tfrac{1}{2} \ln \frac{q^2}{p^2-k^2} + \frac{p+q_z}{2k} \ln \frac{p+k}{p-k} + i\pi \frac{q+q_z}{2q}\right]. \end{aligned} \tag{A. 21}$$

Altogether, we obtain for I_3^1

$$I_3^1 = N a \left[\pi^2 \left(-\frac{\varepsilon-1}{\varepsilon+1} \frac{Y}{X^{\frac{3}{2}}} + \frac{2U}{X^{\frac{1}{2}}}\right) + i\pi \left(R\cos\theta + \frac{2p}{\varepsilon+1} \frac{Y}{X} - 2Z\right)\right]. \tag{A. 22}$$

U and Z are defined in (5.2).

For the first integral in I_6^1 we have in the desired order

$$\int (1 - r^{\gamma-1}) H F\, d\,\mathfrak{r} = \tfrac{1}{2} a^2 \left[\int \ln r \cdot H(\mathfrak{r})\, d\,\mathfrak{r}\right]_{a=0}. \tag{A. 23}$$

The integration over angles is easily performed, and in the integration over r one can rotate the path of integration to the imaginary axis:

$$\int \ln r \cdot H(\mathbf{r})\, d\mathbf{r} = \frac{4\pi}{q} Im \int_0^\infty r \ln r \cdot \exp\left[-(a - iq) r\right] dr = -\frac{2\pi^2}{q^3} + 0(a). \qquad (A.\ 24)$$

The first integral in I_6^1 then gives a contribution

$$N a \pi^2 \frac{2p}{\varepsilon + 1} \frac{1}{X^{\frac{3}{2}}}. \qquad (A.\ 25)$$

I_7^1 and the second integral in I_6^1 are of the form

$$I(f) = \int\int \exp(-ar + i\mathbf{k}\cdot\mathbf{r}) \frac{\exp(ip|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} f(\mathbf{r}')\, d\mathbf{r}\, d\mathbf{r}'. \qquad (A.\ 26)$$

From the Green's function property of $\exp(ip|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|$ it follows that

$$I(f) = -4\pi \int \exp(-ar + i\mathbf{k}\cdot\mathbf{r})\, u(\mathbf{r})\, d\mathbf{r},$$

where $u(\mathbf{r})$ is the solution of $(\Delta + p^2) u = f$, which for large r behaves as an outgoing spherical wave. Using Green's formula, with u as above and $v = \exp(-ar + i\mathbf{k}\cdot\mathbf{r})$, observing that $(\Delta + k^2) v = 0$, apart from terms of order a, we obtain

$$I(f) = -\frac{4\pi}{p^2 - k^2} \int f(\mathbf{r}) \exp(-ar + i\mathbf{k}\cdot\mathbf{r})\, d\mathbf{r} + O(a). \qquad (A.\ 27)$$

This result could also have been established by the use of a suitable Fourier representation of $\exp(ip|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|$.

The integrals in I_6^1 and I_7^1 can now be computed in a way analogous to the earlier computations; no essentially new difficulties arise. The results are

$$I_6^1 = N a \left\{ \pi^2 \left(\frac{2p}{\varepsilon + 1} \frac{1}{X^{\frac{3}{2}}} - \frac{2}{p} \frac{1}{X^{\frac{1}{2}}} + \frac{1}{p^2} \right) + i \left[\frac{\ln \varepsilon (1 + \beta)}{p(\varepsilon - 1)} - \frac{1}{p^2} \ln \varepsilon (1 - \beta \cos \theta) \right] \right\}, \qquad (A.\ 28)$$

$$I_7^1 = N a \sin \theta \left[-\pi^2 U + i\pi \left(\frac{\ln \varepsilon (1 + \beta)}{p^2} - (\varepsilon - 1) Y Z \right) \right]. \qquad (A.\ 29)$$

From the expressions for $I_1^1 \ldots I_7^1$ and the a-order terms in A^0, B^0, C^0 and D^0 we now obtain $A_{1R} \ldots D_{1I}$ in (5.4) and (5.5).

REFERENCES

Banerjee, H., 1958. Nuovo Cim. *10* (1958), p. 863.

——, 1959. Nuovo Cim. *11* (1959), p. 220.

Bethe, H., and Maximon, L. C., 1954. Phys. Rev. *93* (1954), p. 768.

Bethe, H., and Salpeter, E. E., 1957. Handbuch der Physik XXXV. (Springer 1957.)

Brini, D., Peli, L., Rimondi, O., and Veronesi, P., 1957. Nuovo Cim. *6* (1957), p. 98.

Dirac, P. M., 1947. Principles of quantum mechanics. 3rd ed. (Oxford 1947.)

Edmonds, A. R., 1957. Angular momentum in quantum mechanics. (Princeton 1957.)

Erber, T., 1959. Annals of Physics *8* (1959), p. 435.

Fano, U., McVoy, K. W., and Albers, J. R., 1959. Phys. Rev. *116* (1959), p. 1147.

Gavrila, M., 1959. Phys Rev. *113* (1959), p. 514.

——, 1960. Nuovo Cim. *15* (1960), p. 691.

Hulme, H. R., McDougall, J., Buckingham, R. A., and Fowler, R. H., 1935. Proc. Roy. Soc. A *149* (1935), p. 131.

Hultberg, S., 1959. Arkiv f. Fys. *15* (1959), p. 307.

McMaster, W. H., and Hereford, F. L., 1954. Phys. Rev. *95* (1954), p. 723.

McVoy, K. W., 1957. Phys. Rev. *108* (1957). p. 365.

Nagel, B., 1960. Trans. Roy. Inst. Tech., Stockholm. No. 157 (1960).

Nagel, B., and Olsson, P. O. M., 1960. Arkiv f. Fys., following paper.

Nordsieck, A., 1954. Phys. Rev. *93* (1954), p. 785.

Olsen, H., 1958. Kongl. Norske Videnskab. Selsk. Forh. *31* (1958), pp. 61, 66.

Olsson, P. O. M., 1959. Arkiv f. Fys. *15* (1959), pp. 131, 159, 289.

Pratt, R. H., 1960. Phys. Rev. *117* (1960), p. 1017.

Sauter, F., 1931. Ann. Physik *9* (1931), p. 217; *11* (1931), p. 454.

Sauter, F., and Wüster, H. O., 1955. Zeits. f. Physik *141* (1955), p. 83.

Sommerfeld, A., 1939. Atombau und Spektrallinien, Vol. 2 (Wellenmechanik). (Braunschweig 1939.)

Sommerfeld, A., and Maue, A. W., 1935. Ann. Physik *22* (1935), p. 629.

Tolhoek, H. A., 1956. Revs. Modern Phys. *28* (1956), p. 277.

Tryckt den 19 maj 1960

Uppsala 1960. Almqvist & Wiksells Boktryckeri AB